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# MONTE CARLO STUDY OF THE TWO-DIMENSIONAL SPIN-1/2 XY MODEL <sup>☆</sup>

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The generalized Trotter formula is used to map the two-dimensional spin-1/2 XY model onto a three-dimensional Ising model with complicated many-spin interactions. This relationship is used to construct an efficient Monte Carlo algorithm. Simulation data for the specific heat and vortex correlation functions give strong evidence for the existence of a phase transition.

Although it is well known that there cannot exist long-range order in the two-dimensional (2D) spin-1/2 XY model at non-zero temperature [1], high-temperature series expansions [2] suggest the existence of critical behavior. Little is known about the quantum model mainly because most techniques which have been successfully applied to the classical model (also referred to as planar rotator model) are very difficult to extend to the quantum case. In particular, quantum renormalization group analysis of the 2D spin-1/2 XY model have given either contradictory or unreliable results [3–8].

An alternative method to calculate the thermodynamic properties of this model is to exploit the formal analogy between  $d$ -dimensional quantum spin systems and  $(d+1)$ -dimensional Ising-spin models [9]. Using

the generalized Trotter formula [9], Suzuki showed that  $Z = \text{Tr} \exp(-\beta H) = \lim_{m \rightarrow \infty} Z_m$  where

$$Z_m = \text{Tr} \left[ \prod_{\langle ij \rangle} \exp[-(\beta/m) H_{i,j}] \right]^m, \quad (1)$$

is the  $m$ th approximation to the partition function  $Z$ ,  $H_{i,j} = -J(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$ ,  $\sigma_i$  is the Pauli spin-operator at site  $i$  and the product in (1) runs over some ordered set of nearest neighbor bonds of the square lattice. The basic idea of our approach is to calculate the thermodynamic properties of the approximation (1) and to study the convergence of the results as a function of  $m$ . Two of us have already given a rigorous solution of the simplest approximation  $Z_1$  for a large class of orderings and it was shown that in this approximation there is a phase transition of unconventional nature (i.e. no spontaneous magnetization but a logarithmic divergence of the specific heat) [10].

A disadvantage of the special class of exactly solvable  $m=1$  approximations is that the construction [10] that maps them onto staggered 8-vertex models

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[11] is difficult to generalize to  $m > 1$  and, more importantly, it is very difficult and inefficient to perform Monte Carlo simulations with this type of representation. An extensive discussion of the fundamental and technical problems that arise in simulations of 1D spin-1/2 models ( $XY$  and Heisenberg models) can be found in ref. [12].

For the  $d$ -dimensional  $XY$  model we have found representations of (1) that do not suffer from the problems encountered in simulations of 1D spin-1/2 systems [12]. First we note that (1) remains invariant if we rotate all spins over  $\pi/2$  about the  $x$ -axis. Working with the  $XZ$  instead of  $XY$  model solves the problem of constructing algorithms that generate ergodic Markov chains. As this step is essential for the construction of an efficient algorithm, it is clear that our approach for the  $XY$  model cannot be used to study the isotropic Heisenberg system. We partition the hamiltonian in two parts  $H = A + B$  where  $A$  contains all horizontal and  $B$  all vertical bonds. Clearly  $A$  ( $B$ ) is a sum of non-interacting  $XZ$  chains. We obtain an expression of the form (1) by decomposing  $A$  and  $B$  into blocks of two sites. Having specified the ordering in (1) the next step is to introduce complete sets of states between all the exponential factors in (1). As each spin interacts with four neighbors we need  $4mN^2$  ( $N$  is the linear size of the system) Ising-spin variables. To proceed further we calculate the explicit form of the matrix elements of the two-site factors

$$\begin{aligned} \langle S_i S_j | \exp[K_m(\sigma_i^x \sigma_j^x + \sigma_i^z \sigma_j^z)] | \sigma_i \sigma_j \rangle \\ = \delta_{S_i S_j, \sigma_i \sigma_j} (\frac{1}{2} \sinh 2K_m)^{1/2} \\ \times \exp[\bar{K}_m S_i \sigma_j + K_m S_i S_j], \end{aligned} \quad (2)$$

where  $K_m = \beta J/m$ ,  $\bar{K}_m = \frac{1}{2} \ln \coth K_m$ ,  $\sigma_i^z |S_i\rangle = S_i |S_i\rangle$  and  $\sigma_i^x |S_i\rangle = \sigma_i |S_i\rangle$ . Finally we sum out  $2mN^2$  of the Ising spins analytically [13]. In our simulations we have used two different decompositions for the  $XZ$  chains; Suzuki's [9] real-space and Barma and Shastry's [14] checkerboard break-up. For  $m = 1$  we can show that none of these two choices is in the class of orderings that lead to the rigorous  $m = 1$  solution [10]. In the case of the real-space decomposition the final expression for  $Z_m$  reads

$$\begin{aligned} Z_m = c(\sinh 2K_m)^{mN^2} \\ \times \sum'_{\{S_{ij}^{(k)}\}} \sum'_{\{\sigma_{ij}^{(k)}\}} \prod_{k=1}^m \prod_{j=1}^N \prod_{i=1}^N h(j, k) v(i, k), \end{aligned} \quad (3)$$

where for periodic boundary conditions

$$\begin{aligned} h(j, k) = & \cosh[\bar{K}_m(S_{1,j}^{(k)} \sigma_{1,j}^{(k)} + \dots \\ & + S_{1,j}^{(k)} \dots S_{N,j}^{(k)} \sigma_{1,j}^{(k)} \dots \sigma_{N,j}^{(k)}) \\ & + K_m(S_{1,j}^{(k)} S_{2,j}^{(k)} S_{3,j}^{(k)} \sigma_{1,j}^{(k)} + \dots \\ & + S_{1,j}^{(k)} \dots S_{N,j}^{(k)} \sigma_{1,j}^{(k)} \dots \sigma_{N-2,j}^{(k)})] \\ & \times \exp[K_m(S_{1,j}^{(k)} S_{2,j}^{(k)} \\ & + S_{1,j}^{(k)} \dots S_{N,j}^{(k)} \sigma_{2,k}^{(k)} \dots \sigma_{N-1,j}^{(k)})], \end{aligned} \quad (4)$$

$c$  is an unimportant numerical constant and  $v(i, k)$  can be obtained from  $h(j, k)$  by substituting  $S_{i,j}^{(k)} \rightarrow \sigma_{i,j}^{(k)}$  and  $\sigma_{i,j}^{(k)} \rightarrow S_{i,j}^{(k+1)}$ . The 3D lattice model (3), (4) has complicated many-spin interactions and a coupling that depends on the lattice size in the new direction (labeled by the superscript  $k$ ). The checkerboard representation for  $Z_m$  looks similar to (3), (4). As for the 1D case [13] we find that the real-space decomposition converges faster than the checkerboard break-up and therefore we have used the real-space representation for most of our simulation work. The prime on the summation symbols in (3) indicate that the sums over the Ising spin variables are restricted by the  $2N$  constraints  $S_{1,j}^{(k)} \dots S_{N,j}^{(k)} = \sigma_{1,j}^{(k)} \dots \sigma_{N,j}^{(k)}$  and  $\sigma_{i,1}^{(k)} \dots \sigma_{i,N}^{(k)} = S_{i,1}^{(k+1)} \dots S_{i,N}^{(k+1)}$ . We have not been able to remove all constraints originating from conservation laws but we have reduced the number of constraints so drastically that they can be handled extremely efficiently.

An efficient implementation of the Monte Carlo algorithm [15] is possible by working with string variables (products of rows or columns of spins) instead of the spins themselves. Also it is not difficult to construct local spin-flip procedures that can generate ergodic Markov chains of configurations. It is straightforward to write down the explicit form of any kind of correlation function in terms of expectation values of Ising spins. Only because of the high dimensionality of the effective lattice model, the computation time per correlation function is considerable. For instance, inclusion of the code for the vortex correlation (see below) results in an increase of 30%. Especially the calculation of the in-plane susceptibility (not the in-plane correlation function) which requires summation of all correlations of the type  $S_{i,j}^{(k)} S_{i',j'}^{(k')}$  would exhaust our present computational resources. To check the algorithm we studied  $3 \times 3$  systems as a function of  $m$

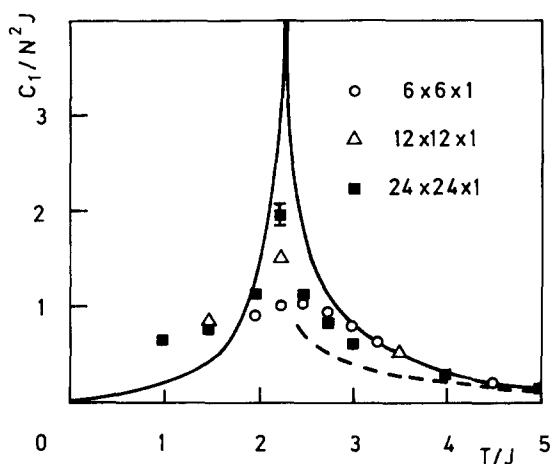


Fig. 1. Specific heat per site of the 2D spin-1/2  $XY$  model in the  $m = 1$  approximation for lattices of different size. Solid line: rigorous staggered 8-vertex solution; broken line: high-temperature expansion. For most temperatures full squares cover open triangles. Statistical errors are of the size of the symbols.

and found excellent agreement with results obtained by summing all terms in (3) and by diagonalizing the full hamiltonian. At high temperatures ( $T \geq 4$ ), our simulation results for the energy and specific heat are in very good agreement with those obtained from high-

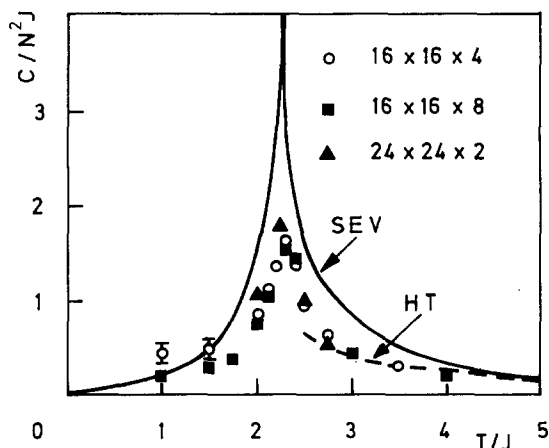


Fig. 2. Specific heat per site of the 2D spin-1/2  $XY$  in the  $m = 1$  approximation. Solid line: rigorous staggered 8-vertex solution; broken line: high-temperature expansion. Comparison with the data of fig. 1 shows that in the critical region the  $m$ -dependence is very weak.

$T$  series [3]. All data presented in this paper have been obtained from at least two independent runs of 10000 Monte Carlo steps per Ising spin each. Simulation of a  $N = 16, m = 8$  ( $16 \times 16 \times 8$ , 4096 Ising spin) system takes 90 min of CPU-time on a CDC 170/750.

Guided by the rigorous  $m = 1$  result (for a different ordering in (1)!) that there is a phase transition at  $\sinh 2K_1^c = 1$ , we first perform simulations for  $m = 1$  for systems of different size. In fig. 1 we depict simulation data for the  $m = 1$  approximant ( $C_1$ ) to the specific heat. At  $K \approx K_1^c$  the specific heat exhibits a maximum that grows slowly with the lattice size. This is in concert with the exact  $m = 1$  solution which predicts a logarithmic divergence of the specific heat [9]. From our  $m = 1$  simulation data we conclude that the phase transition in the  $m = 1$  approximation is not the result of choosing a particular ordering. The first attempt to simulate the 2D  $XY$  model was reported by Suzuki et al. [16] who only studied the  $m = 1$  case. Their simulation data for the specific heat disagree with ours because their algorithm cannot generate ergodic Markov chains of spin states.

The power of our approach is that by increasing  $m$  we can improve approximation (3) systematically. From the  $m > 1$  data shown in fig. 2 we conclude that

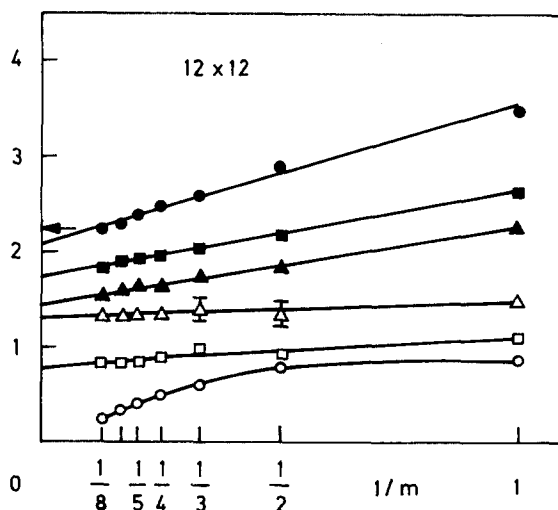


Fig. 3. Minus the energy per site (full symbols) and specific heat per site (open symbols) as a function of  $1/m$  for the  $12 \times 12$  system. Circles:  $T/J = 1$ ; squares:  $T/J = 2$  and triangles  $T/J = 2.25$ . The arrow gives the Pearson's estimate of the ground-state energy.

for  $T/J > 2$  the specific heat, which from the point of view of convergence is the most difficult quantity to calculate [13], depends weakly on the particular value of  $m$ . Except for  $2 \leq T \leq 2.5$  the size dependence of the energy per site and specific heat per site is small. More convincing evidence that the convergence of the energy and specific heat is very good is given in fig. 3. In the critical region ( $T/J \approx 2.27$ ) the  $m$ -dependence of physical quantities is very weak. Therefore it might be tempting to assume that to a good approximation the critical properties of the 2D spin-1/2  $XY$  model are that of the  $m = 1$  representation. Although our numerical data is not inconsistent with this assumption we

take the point of view that the subtle  $\beta/m$  dependence of the approximants could change the critical behavior. Furthermore it is obvious that it is impossible to prove or disprove by means of Monte Carlo data that some physical quantity is continuous or divergent.

To elucidate the nature of the transition we calculate spin-correlation functions which are sensitive to the occurrence of vortex-like excitations. In particular we study the quantum version of Swendsen's vortex detector [17]

$$D = N^{-2} \sum_{\text{plaquettes}} \langle (1 - \sigma_i^x \sigma_k^x - \sigma_i^z \sigma_k^z) \times (1 - \sigma_j^x \sigma_l^x - \sigma_j^z \sigma_l^z) \rangle,$$

where  $i(j)$  and  $k(l)$  label the opposite corners of an elementary square. Simulation data for the approximant  $D_m$  are shown in fig. 4. As for the energy and specific heat the  $m$ -dependence of  $D_m$  is very weak. The rapid change of the disorder-parameter  $D$  as  $K$  approaches  $K_1^c$  strongly suggests that there is a phase transition.

To demonstrate the versatility of our method we have also carried out simulations for systems with  $N = 8, 16$  and  $1 \leq m \leq 32$  for temperatures down to  $T/J = 0.5$ . Within the statistical accuracy of the simulation data (which for the energy is less than one percent), we find that for  $0.5 \leq T/J \leq 1.5$ , the energy is constant. The extrapolated ground state energy per site  $\approx -2.2$  which is in agreement with estimates given by Pearson [18].

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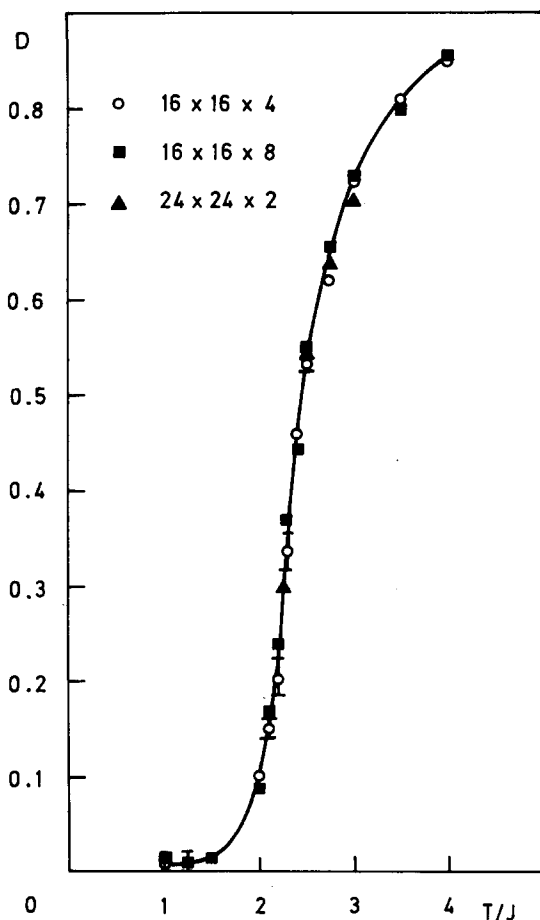


Fig. 4. The vortex correlation function, which measures the degree of disorder in the system, for lattices of different size and different  $m$ . In the critical region the  $m$ -dependence of this correlation function is very weak.

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